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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/694,636	10/27/2003	David E. Patterson	3017-69	3969

7590 01/24/2006
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EXAMINER

ZHOU, SHUBO

ART UNIT PAPER NUMBER

1631

DATE MAILED: 01/24/2006

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary	Application No. 10/694,636	Applicant(s) PATTERSON, DAVID E.	
	Examiner Shubo (Joe) Zhou	Art Unit 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☐ Responsive to communication(s) filed on ____.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 1 is/are pending in the application.
- 4a) Of the above claim(s) ____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) ____ is/are allowed.
- 6) ☒ Claim(s) 1 is/are rejected.
- 7) ☒ Claim(s) 1 is/are objected to.
- 8) ☐ Claim(s) ____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☒ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 27 October 2003 is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
 2. ☐ Certified copies of the priority documents have been received in Application No. ____.
 3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- * See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- | | |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892) | 4) <input type="checkbox"/> Interview Summary (PTO-413)
Paper No(s)/Mail Date. ____. |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | 5) <input type="checkbox"/> Notice of Informal Patent Application (PTO-152) |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08)
Paper No(s)/Mail Date ____. | 6) <input type="checkbox"/> Other: ____. |

DETAILED ACTION

Priority

1. It is noted from the transmittal letter filed 10/27/03 and the declaration under 37 CFR 1.63 filed 8/2/04 that this application appears to claim benefit from prior US application S.N. 09/533,035, filed 3/22/2000. A reference to the prior application must be inserted as the first sentence(s) of the specification of this application or in an application data sheet (37 CFR 1.76), if applicant intends to rely on the filing date of the prior application under 35 U.S.C. 119(e), 120, 121, or 365(c). See 37 CFR 1.78(a). For benefit claims under 35 U.S.C. 120, 121, or 365(c), the reference must include the relationship (i.e., continuation, divisional, or continuation-in-part) of all nonprovisional applications. If the application is a utility or plant application filed under 35 U.S.C. 111(a) on or after November 29, 2000, the specific reference to the prior application must be submitted during the pendency of the application and within the later of four months from the actual filing date of the application or sixteen months from the filing date of the prior application. If the application is a utility or plant application which entered the national stage from an international application filed on or after November 29, 2000, after compliance with 35 U.S.C. 371, the specific reference must be submitted during the pendency of the application and within the later of four months from the date on which the national stage commenced under 35 U.S.C. 371(b) or (f) or sixteen months from the filing date of the prior application. See 37 CFR 1.78(a)(2)(ii) and (a)(5)(ii). This time period is not extendable and a failure to submit the reference required by 35 U.S.C. 119(e) and/or 120, where applicable, within this time period is

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considered a waiver of any benefit of such prior application(s) under 35 U.S.C. 119(e), 120, 121 and 365(c). A benefit claim filed after the required time period may be accepted if it is accompanied by a grantable petition to accept an unintentionally delayed benefit claim under 35 U.S.C. 119(e), 120, 121 and 365(c). The petition must be accompanied by (1) the reference required by 35 U.S.C. 120 or 119(e) and 37 CFR 1.78(a)(2) or (a)(5) to the prior application (unless previously submitted), (2) a surcharge under 37 CFR 1.17(t), and (3) a statement that the entire delay between the date the claim was due under 37 CFR 1.78(a)(2) or (a)(5) and the date the claim was filed was unintentional. The Director may require additional information where there is a question whether the delay was unintentional. The petition should be addressed to: Mail Stop Petition, Commissioner for Patents, P.O. Box 1450, Alexandria, Virginia 22313-1450.

If the reference to the prior application was previously submitted within the time period set forth in 37 CFR 1.78(a), but not in the first sentence(s) of the specification or an application data sheet (ADS) as required by 37 CFR 1.78(a) (e.g., if the reference was submitted in an oath or declaration or the application transmittal letter, as in this instant application), and the information concerning the benefit claim was recognized by the Office as shown by its inclusion on the first filing receipt, the petition under 37 CFR 1.78(a) and the surcharge under 37 CFR 1.17(t) are not required. Applicant is still required to submit the reference in compliance with 37 CFR 1.78(a) by filing an amendment to the first sentence(s) of the specification or an ADS. See MPEP § 201.11.

Specification

2. The specification is objected because of the following:

The arrangement of the specification is confusing. Claims are usually located at the end of the specification. In this case, however, the sheet containing the claim is located before pages 39 and 40, which contain two tables.

It appears that trademark is used in this application, such as OPTISIM on page 27. Trademark should be capitalized wherever it appears and be accompanied by the generic terminology.

Although the use of trademarks is permissible in patent applications, the proprietary nature of the marks should be respected and every effort made to prevent their use in any manner which might adversely affect their validity as trademarks.

Appropriate correction is required.

Claim Objections

3. Claim 1 is objected to because it contains multiple periods, such as those following the step letters a, b, etc. Periods may not be used elsewhere in a claim except for abbreviations.

Where a claim sets forth a plurality of elements or steps, each element or step of the claim should be separated by a line indentation, or by using brackets. See 37 CFR 1.75(I) and MPEP 608.01(m).

Appropriate correction is required.

Claim Rejections-35 USC § 112

4. The following is a quotation of the second paragraph of 35 U.S.C. 112:

The specification shall conclude with one or more claims particularly pointing out and distinctly claiming the subject matter which the applicant regards as his invention.

5. Claim 1 is rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

The following phrases in the claim lack clear antecedent basis and thus make unclear of the metes and bounds of the claim:

“the distance matrix element” in step c.,

“set of compounds” in step d.,

“the first two components” in step e., and

“the initial PCA coordinates” in step f.

The lack of antecedent basis for these limitations renders unclear of the metes and bounds of the claimed invention. For instance, the phrase “the first two PCA components” recited in step (e) lacks clear antecedent basis because there are no PCA components recited prior to the limitation in the claim. It is not clear what components constitute “the first two PCA components”.

The metes and bounds of the “calculating” and “generating” steps (i.e. steps b and c) are unclear. It is not clear from the claim or the specification what procedures are needed to accomplish the steps of “calculating” and “generating.”

The “computing” step (step d)) is vague. It is not clear as to what clusters are calculated, and furthermore, the step has no clear relationship with the prior steps.

The “performing” step (step e)) is vague. It is not clear as to what a PCA is performed on, and the step has no clear relationship with the prior steps.

Step (f), i.e. the step of “using” and “running” is vague. It is not clear what is the relationship thereof with the prior steps. It is also not clear as to what to do using a modified function and on what to run an NLM.

Clarification of the metes and bounds of the claim is requested via clearer claim wording.

It is noted that the claim contains such abbreviations as PCA and NLM, the meaning of which might not be readily apparent to one of ordinary skill in the art. It is suggested that the full terms of such abbreviations be spelled out in the claim.

Claim Rejections-35 USC § 103

6. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

7. Claim 1 is rejected under 35 U.S.C. 103(a) as being unpatentable over Domine et al. (J. Chemometrics, 1993, Vol. 7, pages 227-242) in view of Agrafiotis (J. Chem. Inf. Comput. Sci. 1997, Vol. 37, pages 841-851).

The claim is drawn to a method of visualizing the relationship of compounds in two or three dimensions comprising the steps of: selecting a representative subset of the compounds; calculating or retrieving from a data base the descriptor characteristics for each compound of the subset selected; generating a distance matrix between all compounds or utilizing a function to generate the distance matrix elements as needed; computing a hierarchy of clusters, defining cluster centers and partitioning each set of compounds at each level of clustering; performing a PCA projection onto the first two components; using a modified stress function which reflects a horizon, running an NLM refinement from the initial PCA coordinates; and graphically displaying the coordinates of each compound as determined by the NLM refinement.

Domine et al. disclose methods of non-linear mapping (NLM) for structure-activity and structure-property modeling, comprising selecting a representative subset of compounds of acaricides (page 233, Figure 2) and calculating the molecular descriptor characteristics for each compound (see page 232, especially lines 32-40); generating a matrix (page 233, Table 3); computing a hierarchy of clusters, defining cluster centers and partitioning (page 235); performing a PCA projection onto the components including the first two components, i.e. PC1 and PC2 (pages 234, Figure 4 and page 235); running an NLM refinement from the initial PCA coordinates (page 235, especially lines 9-11 and Figure 5); and graphically displaying the coordinates of each compound as determined by the NLM refinement (page 235, Figure 5, page 236, Figures 6-7, and page 237, Figure 9).

Domine et al. do not explicitly teach using a modified stress function which reflects a horizon.

Agrafiotis discloses a method of maximizing molecular diversity and visualization of results with Sammon's non-linear mapping algorithm comprising using a penalty function (page 844, left column), which function is interpreted as being a stress function required in the instant claim. Agrafiotis teaches that the penalty function consists of overlap penalty and edge penalty wherein if the distance between two points is larger than the sum of the radii of their hyperspheres, the overlap penalty is zero regardless of how far these points are from each other (page 844, right column, first paragraph). This function is interpreted as being the same as the "stress function which reflects a horizon" conceptually and functionally. Agrafiotis states that the function serves to over-penalize close contacts and keep points above some minimum separation and also ensures that the edge effect will not cause the selection algorithm to choose points below some minimum separation that leads to close contacts. This ensures the selection of a well diversified library of compounds. See page 844, right column.

One having ordinary skill in the art would have been motivated at the time the invention was made to modify the method of Domine et al. to include a penalty function points so that points with too close a contact would not be selected ensuring a well diversified library of compounds to be selected.

Double Patenting Rejection

8. The nonstatutory double patenting rejection is based on a judicially created doctrine grounded in public policy (a policy reflected in the statute) so as to prevent the unjustified or improper timewise extension of the "right to exclude" granted by a patent and to prevent possible harassment by multiple assignees. See *In re Goodman*, 11 F.3d 1046, 29 USPQ2d 2010 (Fed.

Cir. 1993); *In re Longi*, 759 F.2d 887, 225 USPQ 645 (Fed. Cir. 1985); *In re Van Ornum*, 686 F.2d 937, 214 USPQ 761 (CCPA 1982); *In re Vogel*, 422 F.2d 438, 164 USPQ 619 (CCPA 1970); and, *In re Thorington*, 418 F.2d 528, 163 USPQ 644 (CCPA 1969).

A timely filed terminal disclaimer in compliance with 37 CFR 1.321(c) may be used to overcome an actual or provisional rejection based on a nonstatutory double patenting ground provided the conflicting application or patent is shown to be commonly owned with this application. See 37 CFR 1.130(b).

Effective January 1, 1994, a registered attorney or agent of record may sign a terminal disclaimer. A terminal disclaimer signed by the assignee must fully comply with 37 CFR 3.73(b).

9. Claim 1 is rejected under the judicially created doctrine of obviousness-type double patenting as being unpatentable over claim 1 of US Patent 6,675,103 ('103).

An obviousness-type double patenting rejection is appropriate where the conflicting claims are not identical, but an examined application claim is not patentably distinct from the reference claims because the examined claim is either anticipated by, or would have been obvious over, the reference claims. See, e.g., *In re Berg*, 140 F.3d 1428, 46 USPQ2d 1226 (Fed. Cir. 1998); *In re Goodman*, 11 F.3d 1046, 29 USPQ2d 2010 (Fed. Cir. 1993); *In re Longi*, 759 F.2d 887, 225 USPQ 645 (Fed. Cir. 1985). Although the conflicting claims are not identical, they are not patentably distinct from each other.

Claim 1 of the instant application is drawn to a method for visualizing the relationship of compounds in high dimensional space comprising selecting a subset of compounds, calculating or retrieving the descriptor characteristics for each compound, generating a distance matrix,

computing a hierarchy of clusters, performing a PCA function, using a stress function and NLM, and graphically displaying the coordinates of each compounds.

While the exact wordings of claim 1 of the '103 patent are not the same as that of claim 1 of the instant application, the only difference in scope is on step b. The step b of claim 1 of the '103 patent requires "evaluating the molecular structural descriptors characteristics of each compound of the subset selected," whereas the step b of the instant claim 1 recites "calculating or retrieving from a database the descriptor characteristics of a compounds." It would have been obvious to one having ordinary skill in the art that "calculating" or "retrieving" descriptor characteristics is certain form of "evaluating" the characteristics. Thus the "evaluating" step of claim 1 of the '103 patent is generic to the "calculating" step of the instant claim 1.

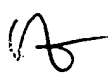
The portion of the specification of the '103 patent that supports the recited "evaluating" procedure includes embodiment that would anticipate the "calculating" step of the instant claim 1. Column 5, lines 1-2 of the '103 patent specifically disclose computing the descriptor characteristics of each compound. Claim 1 of the instant application cannot be considered patentably distinct over claim 1 of the '103 patent when there is a specifically disclosed embodiment in the patent specification that supports claim 1 of that patent and also falls within the scope of the instant claim 1 because it would have been obvious to one having ordinary skill in the art to modify the evaluating step of claim 1 of the '103 patent by selecting a specifically disclosed embodiment that supports the claim, i.e. the "computing" or "calculating" step disclosed in that patent.

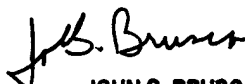
Conclusion

10. No claim is allowed.

11. Any inquiry concerning this communication or earlier communications from the examiner should be directed to Shubo (Joe) Zhou, whose telephone number is 571-272-0724. The examiner can normally be reached Monday-Friday from 8 A.M. to 4 P.M. If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Ardin Marschel, Ph.D., can be reached on 571-272-0718. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300. Any inquiry of a general nature or relating to the status of this application or proceeding should be directed to Patent Analyst Tina Plunkett whose phone number is (571) 272-0549.

Patent applicants with problems or questions regarding electronic images that can be viewed in the Patent Application Information Retrieval system (PAIR) can now contact the USPTO's Patent Electronic Business Center (Patent EBC) for assistance. Representatives are available to answer your questions daily from 6 am to midnight (EST). The toll free number is (866) 217-9197. When calling please have your application serial or patent number, the type of document you are having an image problem with, the number of pages and the specific nature of the problem. The Patent Electronic Business Center will notify applicants of the resolution of the problem within 5-7 business days. Applicants can also check PAIR to confirm that the problem has been corrected. The USPTO's Patent Electronic Business Center is a complete service center supporting all patent business on the Internet. The USPTO's PAIR system provides Internet-based access to patent application status and history information. It also enables applicants to view the scanned images of their own application file folder(s) as well as general patent information available to the public. For all other customer support, please call the USPTO Call Center (UCC) at 800-786-9199.

Shubo (Joe) Zhou, Ph.D. 
Patent Examiner

 20 January 2006
JOHN S. BRUSCA, PH.D.
PRIMARY EXAMINER